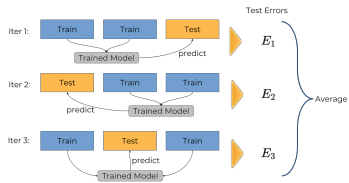


Introduction to Machine Learning

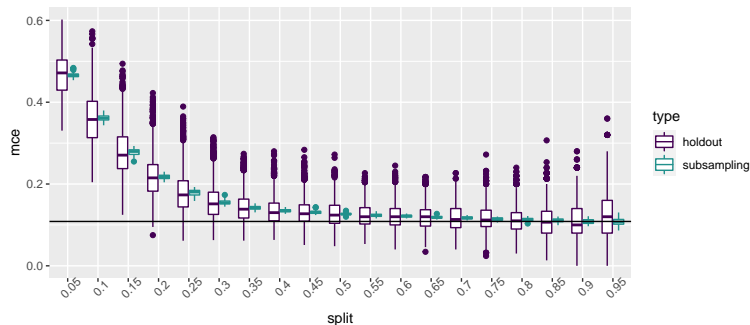
Evaluation Resampling 2



Learning goals

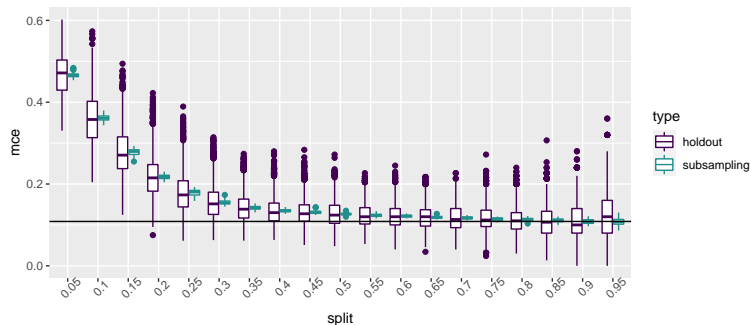
- Understand why resampling is better estimator than hold-out
- In-depth bias-var analysis of resampling estimator
- Understand that CV does not produce independent samples
- Short guideline for practical use

BIAS-VARIANCE ANALYSIS FOR SUBSAMPLING



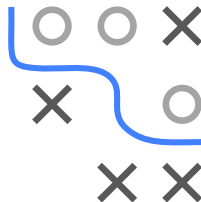
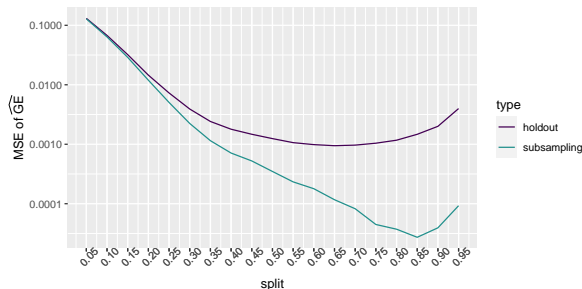
- Reconsider bias-var experiment for holdout (maybe re-read)
- Split rates $s \in \{0.05, 0.1, \dots, 0.95\}$ with $|\mathcal{D}_{\text{train}}| = s \cdot 500$.
- Holdout vs. subsampling with 50 iters
- 50 replications

BIAS-VARIANCE ANALYSIS FOR SUBSAMPLING



- Both estimators are compared to "real" MCE (black line)
- SS same pessimistic bias as holdout for given s , but much less var

BIAS-VARIANCE ANALYSIS FOR SUBSAMPLING



- MSE of \widehat{GE} strictly better for SS
- Smaller var of SS enables to use larger s for optimal choice
- The optimal split rate now is a higher $s \approx 0.8$.
- Beyond $s = 0.8$: MSE goes up because var doesn't go down as much as we want due to increasing overlap in trainsets (see later)

DEDICATED TESTSET SCENARIO - ANALYSIS

- Goal: estimate $\text{GE}(\hat{f}) = \mathbb{E} [L(y, \hat{f}(\mathbf{x}))]$ via

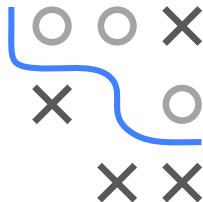
$$\widehat{\text{GE}}(\hat{f}) = \frac{1}{m} \sum_{(\mathbf{x}, y) \in \mathcal{D}_{\text{test}}} L(y, \hat{f}(\mathbf{x}))$$

Here, only (\mathbf{x}, y) are random, they are m i.i.d. fresh test samples

- This is: average over i.i.d $L(y, \hat{f}(\mathbf{x}))$, so directly know \mathbb{E} and var.

And can use CLT to approx distrib of $\widehat{\text{GE}}(\hat{f})$ with Gaussian.

- $\mathbb{E}[\widehat{\text{GE}}(\hat{f})] = \mathbb{E}[L(y, \hat{f}(\mathbf{x}))] = \text{GE}(\hat{f})$
- $\mathbb{V}[\widehat{\text{GE}}(\hat{f})] = \frac{1}{m} \mathbb{V}[L(y, \hat{f}(\mathbf{x}))]$
- So $\widehat{\text{GE}}(\hat{f})$ is unbiased estimator of $\text{GE}(\hat{f})$, var decreases linearly in testset size, have an approx of full distrib (can do NHST, CIs, etc.)
- NB: Gaussian may work less well for e.g. 0-1 loss, with \mathbb{E} close to 0, can use binomial or other special approaches for other losses



PESSIMISTIC BIAS IN RESAMPLING

- Estim $\text{GE}(\mathcal{I}, n)$ (surrogate for $\text{GE}(\hat{f})$) when \hat{f} is fit on full \mathcal{D} , with $|\mathcal{D}| = n$) via resampling based estim $\widehat{\text{GE}}(\mathcal{I}, n_{\text{train}})$

$$\begin{aligned}\widehat{\text{GE}}(\mathcal{I}, \mathcal{J}, \rho, \lambda) &= \text{agr} \left(\rho \left(\mathbf{y}_{J_{\text{test},1}}, \mathbf{F}_{J_{\text{test},1}, \mathcal{I}(\mathcal{D}_{\text{train},1}, \lambda)} \right), \right. \\ &\quad \vdots \\ &\quad \left. \rho \left(\mathbf{y}_{J_{\text{test},B}}, \mathbf{F}_{J_{\text{test},B}, \mathcal{I}(\mathcal{D}_{\text{train},B}, \lambda)} \right) \right),\end{aligned}$$

- Let's assume agr is avg and ρ is loss-based, so ρ_L
- The ρ are simple holdout estims. So:

$$\mathbb{E}[\widehat{\text{GE}}(\mathcal{I}, \mathcal{J}, \rho, \lambda)] \approx \mathbb{E}[\rho(\mathbf{y}_{J_{\text{test}}}, \mathbf{F}_{J_{\text{test}}, \mathcal{I}(\mathcal{D}_{\text{train}}, \lambda)})]$$

- NB1: In above, as always for $\text{GE}(\mathcal{I})$, both $\mathcal{D}_{\text{train}}$ and $\mathcal{D}_{\text{test}}$ (and so $\mathbf{x} \in \mathcal{D}_{\text{test}}$) are random vars, and we take \mathbb{E} over them
- NB2: Need \approx as maybe not all train/test sets in resampling of exactly same size



PESSIMISTIC BIAS IN RESAMPLING / 2

$$\mathbb{E}[\widehat{\text{GE}}(\mathcal{I}, \mathcal{J}, \rho, \lambda)] \approx \mathbb{E}[\rho(\mathbf{y}_{J_{\text{test}}}, \mathbf{F}_{J_{\text{test}}, \mathcal{I}(\mathcal{D}_{\text{train}}, \lambda)})] =$$
$$\mathbb{E} \left[\frac{1}{m} \sum_{(\mathbf{x}, y) \in \mathcal{D}_{\text{test}}} L(y, \mathcal{I}(\mathcal{D}_{\text{train}})(\mathbf{x})) \right] = \text{GE}(\mathcal{I}, n_{\text{train}})$$

\Rightarrow

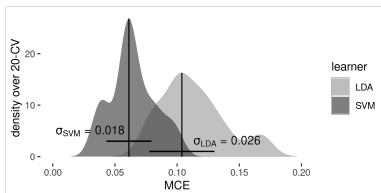
- So when we use $\widehat{\text{GE}}(\mathcal{I}, \mathcal{J}, \rho, \lambda)$ to estimate $\text{GE}(\mathcal{I}, n)$, our expected value is nearly correct, it's $\text{GE}(\mathcal{I}, n_{\text{train}})$
- But fitting \mathcal{I} on less data (n_{train} vs full n) usually results in model with worse perf, hence estimator is pessimistically biased
- Bias the stronger, the smaller our training splits in resampling.



NO INDEPENDENCE OF CV RESULTS

- Similar analysis as before holds for CV
- Might be tempted to report distribution or SD of individual CV split perf values, e.g. to test if perf of 2 learners is significantly different
- But k CV splits are not independent

A t-test on the difference of the mean GE estimators yields a highly significant p-value of $\approx 7.9 \cdot 10^{-5}$ on the 95% level.

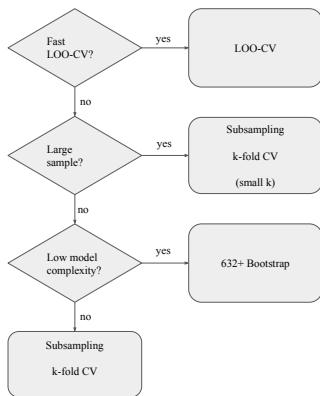


LDA vs SVM on spam classification problem, performance estimation via 20-CV w.r.t. MCE.

NO INDEPENDENCE OF CV RESULTS

- $\mathbb{V}[\widehat{GE}]$ of CV is a difficult combination of
 - average variance as we estim on finite trainsets
 - covar from test errors, as models result from overlapping trainsets
 - covar due to the dependence of trainsets and test obs appear in trainsets
- Naively using the empirical var of k individual \widehat{GE} s (as on slide before) yields biased estimator of $\mathbb{V}[\widehat{GE}]$. Usually this underestimates the true var!
- Worse: there is no unbiased estimator of $\mathbb{V}[\widehat{GE}]$ [Bengio, 2004]
- Take into account when comparing learners by NHST
- Somewhat difficult topic, we leave it with the warning here

SHORT GUIDELINE



- 5-CV or 10-CV have become standard.
- Do not use hold-out, CV with few folds, or SS with small split rate for small n . Can bias estim and have large var.
- For small n , e.g. $n < 200$, use LOO or, probably better, repeated CV.
- For some models, fast tricks for LOO exist
- With $n = 100.000$, can have "hidden" small-sample size, e.g. one class very small
- SS usually better than bootstrapping. Repeated obs can cause problems in training, especially in nested setups where the "training" set is split up again.